Lecture XXI: Cooper instability

In the final section of the course, we will explore a pairing instability of the electron gas which leads to condensate formation and the phenomenon of superconductivity.

▷ History:

- 1911 discovery of superconductivity (Onnes)
- 1951 "isotope effect" — clue to (conventional) mechanism
- 1956 Development of (correct) phenomenology (Ginzburg-Landau)
- 1957 BCS theory of conventional superconductivity (Bardeen-Cooper-Schrieffer)
- 1976 Discovery of unconventional superconductivity in heavy fermions (Steglich)
- 1986 Discovery of high temperature superconductivity in cuprates (Bednorz-Müller)
- ???? awaiting theory?

▷ (Conventional) mechanism: exchange of phonons can induce (space-nonlocal) attractive pairwise interaction between electrons

$$\hat{H}' = \hat{H}_0 - |M|^2 \sum_{\mathbf{k}\mathbf{k}'\mathbf{q}} \frac{\hbar\omega_{\mathbf{q}}}{\hbar^2\omega_{\mathbf{q}}^2 - (\epsilon_{\mathbf{k}} - \epsilon_{\mathbf{k}-\mathbf{q}})^2} c^\dagger_{\mathbf{k}-\mathbf{q}\sigma} c^\dagger_{\mathbf{k}'+\mathbf{q}\sigma'} c_{\mathbf{k}'\sigma'} c_{\mathbf{k}\sigma}$$

Physically electrons can lower their energy by sharing lattice polarisation of another

By exploiting interaction, electron pairs can condense into macroscopic phase coherent state with energy gap to quasi-particle excitations

To understand why, let us consider the argument marshalled by Cooper which lead to the development of a consistent many-body theory.

▷ <u>Cooper instability</u>

Consider two electrons propagating above a filled Fermi sea:
Is a weak pairwise interaction $V(\mathbf{r}_1 - \mathbf{r}_2)$ sufficient to create a bound state?

Consider variational state

$$\psi(\mathbf{r}_1, \mathbf{r}_2) = \overbrace{\frac{1}{\sqrt{2}}(|\uparrow_1\rangle \otimes |\downarrow_2\rangle - |\uparrow_2\rangle \otimes |\downarrow_1\rangle)}^{\text{spin singlet}} \overbrace{\sum_{|\mathbf{k}|\geq k_F} g_{\mathbf{k}} e^{i\mathbf{k}\cdot(\mathbf{r}_1-\mathbf{r}_2)}}^{\text{spatial symm. } g_{\mathbf{k}} = g_{-\mathbf{k}}}$$

Applied to Schrödinger equation: $\hat{H}\psi = E\psi$

$$\sum_{\mathbf{k}} g_{\mathbf{k}} \left[2\epsilon_{\mathbf{k}} + V(\mathbf{r}_1 - \mathbf{r}_2)\right] e^{i\mathbf{k}\cdot(\mathbf{r}_1-\mathbf{r}_2)} = E \sum_{\mathbf{k}} g_{\mathbf{k}} e^{i\mathbf{k}\cdot(\mathbf{r}_1-\mathbf{r}_2)}$$

Fourier transforming equation: $\times L^{-d}\int d(\mathbf{r}_1-\mathbf{r}_2)e^{-i\mathbf{k}'\cdot(\mathbf{r}_1-\mathbf{r}_2)}$

$$\sum_{\mathbf{k}'} V_{\mathbf{k}-\mathbf{k}'}g_{\mathbf{k}'} = (E-2\epsilon_{\mathbf{k}})g_{\mathbf{k}}, \qquad V_{\mathbf{k}\mathbf{k}'} = \frac{1}{L^d}\int d\mathbf{r}\, V(\mathbf{r})e^{i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{r}}$$

If we assume $V_{\mathbf{k}-\mathbf{k}'} = \begin{cases} -\frac{V}{L^d} & \{|\epsilon_{\mathbf{k}}-\epsilon_F|, |\epsilon_{\mathbf{k}'}-\epsilon_F|\} < \omega_D \\ 0 & \text{otherwise}\end{cases}$

$$-\frac{V}{L^d}\sum_{\mathbf{k}'} g_{\mathbf{k}'} = (E-2\epsilon_{\mathbf{k}})g_{\mathbf{k}} \mapsto -\frac{V}{L^d}\sum_{\mathbf{k}}\frac{1}{E-2\epsilon_{\mathbf{k}}}\sum_{\mathbf{k}'} g_{\mathbf{k}'} = \sum_{\mathbf{k}} g_{\mathbf{k}} \mapsto -\frac{V}{L^d}\sum_{\mathbf{k}}\frac{1}{E-2\epsilon_{\mathbf{k}}} = 1$$

Using $\displaystyle \frac{1}{L^d}\sum_{\mathbf{k}} = \int \frac{d^dk}{(2\pi)^d} = \int \nu(\epsilon)\,d\epsilon \sim \nu(\epsilon_F)\int d\epsilon$, where $\displaystyle \nu(\epsilon) = \frac{1}{|\partial_{\mathbf{k}}\epsilon_{\mathbf{k}}|}$ is DoS

$$\frac{V}{L^d}\sum_{\mathbf{k}}\frac{1}{2\epsilon_{\mathbf{k}}-E} \simeq \nu(\epsilon_F)V\int_{\epsilon_F}^{\epsilon_F+\omega_D}\frac{d\epsilon}{2\epsilon-E} = \frac{\nu(\epsilon_F)V}{2}\ln\left(\frac{2\epsilon_F+2\omega_D-E}{2\epsilon_F-E}\right) = 1$$

In limit of weak coupling, i.e. $\nu(\epsilon_F)V \ll 1$

$$E \simeq 2\epsilon_F - 2\omega_D e^{-\frac{2}{\nu(\epsilon_F)V}}$$

- i.e. pair forms a bound state (no matter how small interaction!)
- energy of bound state is non-perturbative in $\nu(\epsilon_F)V$

▷ Radius of pair wavefunction: $g(\mathbf{r}) = \sum_{\mathbf{k}} g_{\mathbf{k}}e^{i\mathbf{k}\cdot\mathbf{r}}$, $g_{\mathbf{k}} = \frac{1}{2\epsilon_{\mathbf{k}}-E}\times$ const., $\partial_{\mathbf{k}} = \frac{\partial\epsilon_{\mathbf{k}}}{\partial\mathbf{k}}\frac{\partial}{\partial\epsilon}$

$$\langle\mathbf{r}^2\rangle = \frac{\int d^dr\ \mathbf{r}^2|g(\mathbf{r})|^2}{\int d^dr|g(\mathbf{r})|^2} = \frac{\sum_{\mathbf{k}}|\partial_{\mathbf{k}}g_{\mathbf{k}}|^2}{\sum_{\mathbf{k}}|g_{\mathbf{k}}|^2} \simeq \frac{v_F^2\int_{\epsilon_F}^{\epsilon_F+\omega_D}\frac{4d\epsilon}{(2\epsilon-E)^4}}{\int_{\epsilon_F}^{\epsilon_F+\omega_D}\frac{d\epsilon}{(2\epsilon-E)^2}} = \frac{4}{3}\frac{v_F^2}{(2\epsilon_F-E)^2}$$

if binding energy $2\epsilon_F - E \sim k_{\mathrm{B}}T_c$, $T_c \sim 10\mathrm{K}$, $v_F \sim 10^8\mathrm{cm/s}$, $\xi_0 = \langle\mathbf{r}^2\rangle^{1/2} \sim 10^4\mathring{A}$,
i.e. other electrons must be important

▷ BCS WAVEFUNCTION

Two electrons in a paired state has wavefunction

$$\phi(\mathbf{r}_1-\mathbf{r}_2) = (|\uparrow_1\rangle\otimes|\downarrow_2\rangle - |\downarrow_1\rangle\otimes|\uparrow_2\rangle)g(\mathbf{r}_1-\mathbf{r}_2)$$

with zero centre of mass momentum

Drawing analogy with Bose condensate, let us examine variational state

$$\psi(\mathbf{r}_1\cdots\mathbf{r}_{2N}) = \mathcal{N}\prod_{n=1}^{N}\phi(\mathbf{r}_{2n-1}-\mathbf{r}_{2n})$$

Is state compatible with Pauli principle? Using $g(\mathbf{r}_1 - \mathbf{r}_2) = \sum_{\mathbf{k}} g_{\mathbf{k}} e^{i\mathbf{k}\cdot(\mathbf{r}_1-\mathbf{r}_2)}$
or, in Fourier representation

$$\int \frac{d^d r_1}{L^d} e^{-i\mathbf{k}_1\cdot\mathbf{r}_1} \int \frac{d^d r_2}{L^d} e^{-i\mathbf{k}_2\cdot\mathbf{r}_2} g(\mathbf{r}_1 - \mathbf{r}_2) = \sum_{\mathbf{k}} g_{\mathbf{k}} \delta_{\mathbf{k}_1,\mathbf{k}} \delta_{\mathbf{k}_2,-\mathbf{k}}$$

or in second quantised form,

$$\mathrm{FT}\left[g(\mathbf{r}_1 - \mathbf{r}_2) c^\dagger_\uparrow(\mathbf{r}_1) c^\dagger_\downarrow(\mathbf{r}_2)|\Omega\rangle\right] = \sum_{\mathbf{k}} g_{\mathbf{k}}\, c^\dagger_{\mathbf{k}\uparrow} c^\dagger_{-\mathbf{k}\downarrow}|\Omega\rangle$$

Then, of the terms in the expansion of

$$|\psi\rangle = \prod_{n=1}^{N}\left[\sum_{\mathbf{k}_n} g_{\mathbf{k}_n} c^\dagger_{\mathbf{k}_n\uparrow} c^\dagger_{-\mathbf{k}_n\downarrow}\right]|\Omega\rangle$$

those with all $\mathbf{k}_n$s different survive

Generally, more convenient to work in grand canonical ensemble
where one allows for (small) fluctuations in the total particle density

$$|\psi\rangle = \prod_{\mathbf{k}} (u_{\mathbf{k}} + v_{\mathbf{k}} c^\dagger_{\mathbf{k}\uparrow} c^\dagger_{-\mathbf{k}\downarrow})|\Omega\rangle \ \sim \overbrace{\exp\left[\sum_{\mathbf{k}} g_{\mathbf{k}} c^\dagger_{\mathbf{k}\uparrow} c^\dagger_{-\mathbf{k}\downarrow}\right]|\Omega\rangle}^{\text{cf. coherent state}}$$

i.e. statistical independence of pair occupation

In non-interacting electron gas $v_{\mathbf{k}} = \begin{cases} 1 & |\mathbf{k}| < k_F \\ 0 & |\mathbf{k}| > k_F \end{cases}$

In interacting system, to determine the variational parameters $v_{\mathbf{k}}$,
one can use a variational principle, i.e. to minimise

$$\langle\psi|\hat{H} - \epsilon_F \hat{N}|\psi\rangle$$

▷ BCS Hamiltonian

However, since we are interested in both the ground state energy, and the spectrum of quasi-particle excitations, we will follow a different route and explore a simplified model Hamiltonian

$$\hat{H} = \sum_{\mathbf{k}} \epsilon_{\mathbf{k}} c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} - V \sum_{\mathbf{k}\mathbf{k}'} c^\dagger_{\mathbf{k}'\uparrow} c^\dagger_{-\mathbf{k}'\downarrow} c_{-\mathbf{k}\downarrow} c_{\mathbf{k}\uparrow}$$